Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	2516	Alonso-Alija.in. or Heil.in. or Flubacher.in. or Naab.in. or Stasch.in. or Wunder.in. or Dembowsky.in. or Perzborn.in. or Stahl.in.	US-PGPUB; USPAT	OR	OFF	2005/10/31 14:06
L2	7	l1 and dicarboxylic.clm.	US-PGPUB; USPAT	OR	OFF	2005/10/31 14:07

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=> d his

     (FILE 'HOME' ENTERED AT 10:40:23 ON 31 OCT 2005)

     FILE 'REGISTRY' ENTERED AT 10:40:33 ON 31 OCT 2005
L1                STRUCTURE UPLOADED
L2              4 S L1 SSS
L3                STRUCTURE UPLOADED
L4              2 S L3 SSS
L5                STRUCTURE UPLOADED
L6              1 S L5 SSS
L7                STRUCTURE UPLOADED
L8              1 S L7 SSS
L9            168 S L7 SSS FULL

     FILE 'CAPLUS' ENTERED AT 10:45:09 ON 31 OCT 2005
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L11               STRUCTURE UPLOADED
                  S L11

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L12             0 S L11 SSS

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L13             0 S L12 SSS

     FILE 'REGISTRY' ENTERED AT 10:51:55 ON 31 OCT 2005
L14               STRUCTURE UPLOADED
L15             0 S L14 SSS
L16               STRUCTURE UPLOADED
L17             0 S L16 SSS
L18            23 S L16 SSS FULL

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=> d l16
L16 HAS NO ANSWERS
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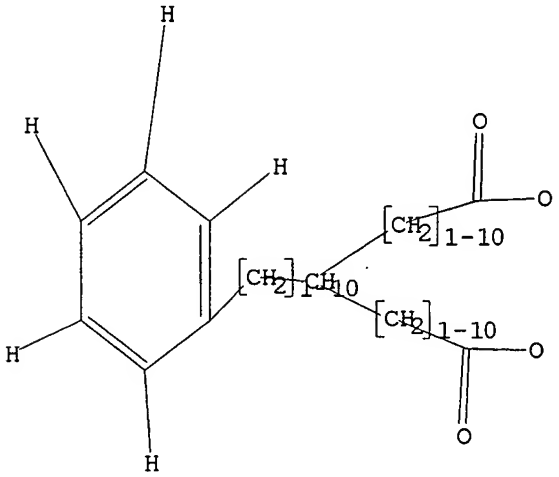
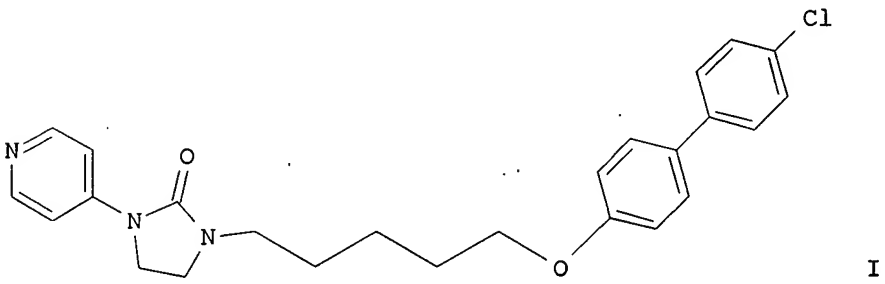


Structure attributes must be viewed using STN Express query preparation.

=> d bib abs hitstr 1-15

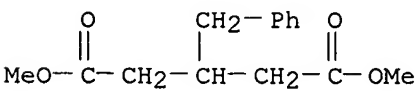
L19 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:331777 CAPLUS
DN 143:43827
TI Design, Synthesis, and Antipicornavirus Activity of 1-[5-(4-Arylphenoxy)alkyl]-3-pyridin-4-ylimidazolidin-2-one Derivatives
AU Chang, Chih-Shiang; Lin, Ying-Ting; Shih, Shin-Ru; Lee, Chung-Chi; Lee, Yen-Chun; Tai, Chia-Liang; Tseng, Sung-Nien; Chern, Jyh-Haur
CS Division of Biotechnology and Pharmaceutical Research, National Health Research Institutes, Zhunan, 350, Taiwan
SO Journal of Medicinal Chemistry (2005), 48(10), 3522-3535
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



I

AB A series of pyridylimidazolidinone derivs. was synthesized and tested in vitro against enterovirus 71 (EV71). On the basis of DBPR103 (I), introduction of a Me group at the 2- or 3-position of the linker between the imidazolidinone and the biphenyl resulted in markedly improved antiviral activity toward EV71 with IC50 values of 5.0 nM and 9.3 nM, resp. Increasing the branched chain to Pr resulted in a progressive decrease in activity, while inserting different heteroatoms entirely rendered the compound only weakly active. The introduction of a bulky group (cyclohexyl, Ph, or benzyl) led to loss of activity against EV71. The 4-chlorophenyl moiety was replaced with bioisosteric groups such as oxadiazole or tetrazole dramatically improving anti-EV71 activity and selectivity indexes. Some of these compds. exhibited a strong activity against lethal EV71, and no apparent cellular toxicity was observed Three of the more potent imidazolidinone compds. were subjected to a large group of picornaviruses to determine their spectrum of antiviral activity.

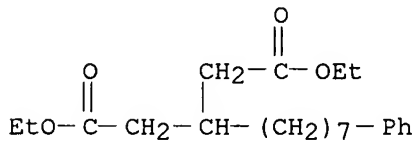
IT **91478-80-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and antienterovirus 71 activity of 1-[5-(4-arylphenoxy)alkyl]-3-pyridin-4-ylimidazolidin-2-one derivs.)
RN 91478-80-7 CAPLUS
CN Pentanedioic acid, 3-(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RE.CNT 96 THERE ARE 96 CITED REFERENCES AVAILABLE FOR THIS RECORD

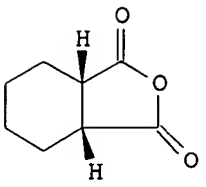
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L19 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:46609 CAPLUS
DN 130:252502
TI Zwitterionic sulfobetaine inhibitors of squalene synthase
AU Spencer, Thomas A.; Onofrey, Thomas J.; Cann, Reginald O.; Russel, Jonathon S.; Lee, Laura E.; Blanchard, Daniel E.; Castro, Alfredo; Gu, Peide; Jiang, Guojian; Shechter, Ishaiahu
CS Department of Chemistry, Dartmouth College, Hanover, NH, 03755, USA
SO Journal of Organic Chemistry (1999), 64(3), 807-818
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
OS CASREACT 130:252502
AB A number of sulfobetaines were synthesized and evaluated as inhibitors of squalene synthase (SS) on the basis of the idea that their zwitterionic structure would have properties conducive both to binding in the active site and to passage through cell membranes. When the simple sulfobetaine moiety is incorporated into compds. containing hydrophobic portions like those in farnesyl diphosphate or presqualene diphosphate, inhibition of SS in a rat liver microsomal assay was indeed observed A wide variety of structural modifications was investigated. Unfortunately, no inhibitors in the submicromolar range were discovered, and exploration of a different type of zwitterion seems necessary if this appealing approach to inhibition of SS is going to provide a potential antihypercholesterolemic agent.
IT **221657-07-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of zwitterionic sulfobetaine inhibitors of squalene synthase)
RN 221657-07-4 CAPLUS
CN Pentanedioic acid, 3-(7-phenylheptyl)-, diethyl ester (9CI) (CA INDEX NAME)

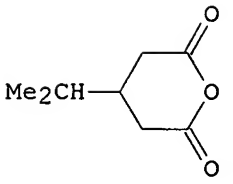


RE.CNT 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

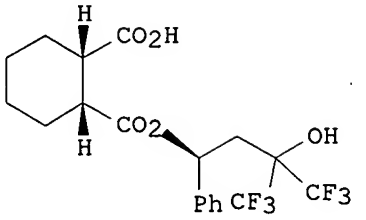
L19 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:235392 CAPLUS
DN 116:235392
TI Highly diastereoselective alcoholysis of σ-symmetric dicarboxylic acid anhydrides using 1-phenyl-3,3-bis(trifluoromethyl)propane-1,3-diol
AU Suda, Yoshimitsu; Yago, Seiji; Shiro, Motoo; Taguchi, Takeo
CS Tokyo Coll. Pharm., Hachioji, 192-03, Japan
SO Chemistry Letters (1992), (3), 389-92
CODEN: CMLTAG; ISSN: 0366-7022
DT Journal
LA English
OS CASREACT 116:235392
GI



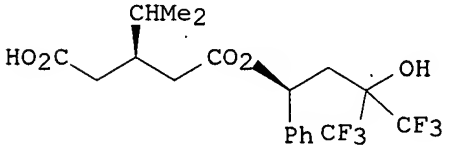
I



II



III



IV

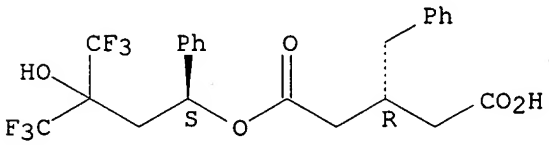
AB Highly diastereoselective alcoholysis of σ-sym. dicarboxylic acid anhydrides, e.g., I and II, was performed using 1-phenyl-3,3-bis(trifluoromethyl)propane-1,3-diol to give chiral half acid esters, e.g., III and IV. The importance of the geminally trifluoromethylated carbinol moiety for achieving a high degree of chiral induction was confirmed from lower diastereoselectivity with the hydroxyl protected 1,3-diol or with the similar 1,3-diols having hydrocarbon substituents instead of the trifluoromethyl group.

IT **141329-91-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and lactonization of)

RN 141329-91-1 CAPLUS

CN Pentanedioic acid, 3-(phenylmethyl)-, mono[4,4,4-trifluoro-3-hydroxy-1-phenyl-3-(trifluoromethyl)butyl] ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:586743 CAPLUS

DN 109:186743

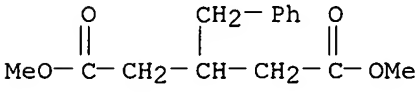
TI Construction of novel chiral synthons with enzymes and application to natural product synthesis. Part 23. Enantioselective hydrolysis of dialkyl 3-monosubstituted glutarates with pig liver esterase: structure-optical purity relationships

AU Nakada, Masahisa; Kobayashi, Susumu; Ohno, Masaji; Iwasaki, Shigeo; Okuda, Shigenobu

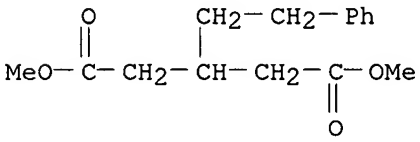
CS Fac. Pharm. Sci., Univ. Tokyo, Tokyo, 113, Japan

SO Tetrahedron Letters (1988), 29(32), 3951-4

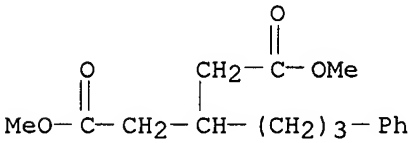
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
OS CASREACT 109:186743
AB Dialkyl 3-monosubstituted glutarates are subjected to hydrolysis with pig liver esterase to afford the corresponding chiral half-esters. Synthetically useful half-esters of higher optical purity are obtained from the prochiral substrates of more hydrophobic nature.
IT **91478-80-7 117213-94-2 117213-97-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective hydrolysis of, with pig liver esterase)
RN 91478-80-7 CAPLUS
CN Pentanedioic acid, 3-(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 117213-94-2 CAPLUS
CN Pentanedioic acid, 3-(2-phenylethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

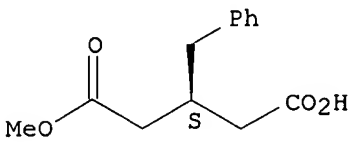


RN 117213-97-5 CAPLUS
CN Pentanedioic acid, 3-(3-phenylpropyl)-, dimethyl ester (9CI) (CA INDEX NAME)



IT **101713-11-5P 117214-01-4P 117214-03-6P**
RL: PREP (Preparation)
(preparation of, from dialkyl glutarate enantioselective hydrolysis with pig liver esterase)
RN 101713-11-5 CAPLUS
CN Pentanedioic acid, 3-(phenylmethyl)-, monomethyl ester, (S)- (9CI) (CA INDEX NAME)

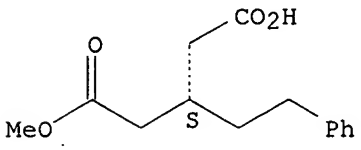
Absolute stereochemistry.



RN 117214-01-4 CAPLUS

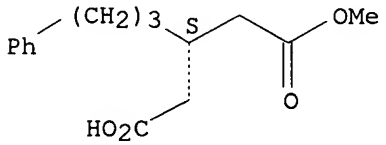
CN Pentanedioic acid, 3-(2-phenylethyl)-, monomethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

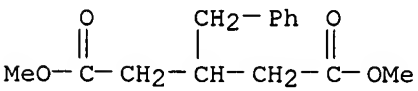


RN 117214-03-6 CAPLUS
CN Pentanedioic acid, 3-(3-phenylpropyl)-, monomethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



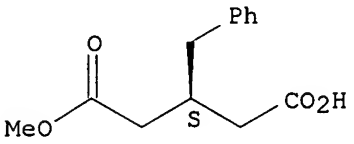
L19 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1986:224741 CAPLUS
DN 104:224741
TI Enzymes in organic synthesis. 35. Stereoselective pig liver esterase catalyzed hydrolyses of 3-substituted glutarate diesters. Optimization of enantiomeric excess via reaction conditions control
AU Lam, Lister K. P.; Hui, Raymond A. H. F.; Jones, J. Bryan
CS Dep. Chem., Univ. Toronto, Toronto, ON, M5S 1A1, Can.
SO Journal of Organic Chemistry (1986), 51(11), 2047-50
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 104:224741
AB Pig liver esterase-catalyzed hydrolyses of RCH(CH2CO2Me)2 (R = Me, Et, Pr, CHMe2, cyclohexyl, Ph, Ch2Ph) are enantiotopically selective, giving (R)-HO2CCH2CHRCH2CO2Me (I, R = Me, Et, Pr, cyclohexyl) and (S)-I (R = CHMe2, Ph, CH2Ph) with enantiomeric excess under normal aqueous hydrolysis conditions. The stereoselectivity was increased by adding 20% MeOH. An active site model consistent with these data is presented.
IT **91478-80-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective ester hydrolysis of, with esterase)
RN 91478-80-7 CAPLUS
CN Pentanedioic acid, 3-(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



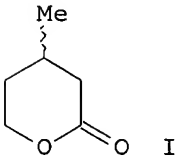
IT **101713-11-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective preparation of, by esterase hydrolysis of diester)
RN 101713-11-5 CAPLUS
CN Pentanedioic acid, 3-(phenylmethyl)-, monomethyl ester, (S)- (9CI) (CA

INDEX NAME)

Absolute stereochemistry.

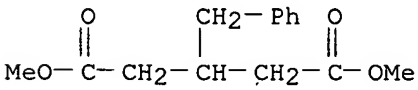


L19 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1984:490720 CAPLUS
DN 101:90720
TI Preparations of chiral δ-lactones via enantiotopically specific pig liver esterase-catalyzed hydrolyses of 3-substituted glutaric acid diesters
AU Francis, Christopher J.; Jones, Bryan J.
CS Dep. Chem., Univ. Toronto, Toronto, M5S 1A1, Can.
SO Journal of the Chemical Society, Chemical Communications (1984), (9), 579-80
CODEN: JCCCAT; ISSN: 0022-4936
DT Journal
LA English
OS CASREACT 101:90720
GI



I

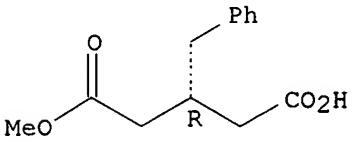
AB Pig liver esterase-catalyzed hydrolyses of 3-monosubstituted glutaric acid diesters were pro-S enantiospecific for a variety of substituents, allowing the preparation of either enantiomer of the corresponding 3-substituted valerolactone in an optically pure form. E.g., hydrolysis of MeCH(CH2CO2Me)2 with pig liver esterase at pH 7 gave 98% (3R)-HO2CCH2CHMeCH2CO2Me which was selectively reduced by BH3.Me2S or LiBH4 to give lactones (+)-(4R)- and (-)-(4S)-I, resp., in 86% yield.
IT **91478-80-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, by pig liver esterase)
RN 91478-80-7 CAPLUS
CN Pentanedioic acid, 3-(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



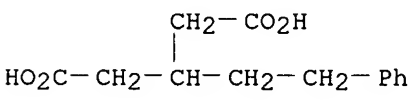
IT **91478-86-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and selective reduction of, lactones by)
RN 91478-86-3 CAPLUS
CN Pentanedioic acid, 3-(phenylmethyl)-, monomethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

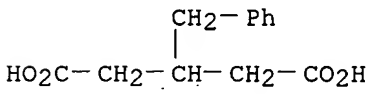


L19 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1979:523603 CAPLUS
DN 91:123603
TI Enzymes in organic synthesis. 14. Stereoselective horse liver alcohol dehydrogenase catalyzed oxidations of diols containing a prochiral center and of related hemiacetals
AU Jones, J. Bryan; Lok, Kar P.
CS Dep. Chem., Univ. Toronto, Toronto, ON, M5S 1A1, Can.
SO Canadian Journal of Chemistry (1979), 57(9), 1025-32
CODEN: CJCHAG; ISSN: 0008-4042
DT Journal
LA English
OS CASREACT 91:123603
AB The title oxidns. of 3-substituted pentane-1,5-diols proceed with enantiotropic selectivity to give ≤78% enantiomeric excess of 3S-3-substituted valerolactones. Initial oxidation of the pro-S hydroxyethyl group gave hydroxyaldehydes which undergo in situ enzyme-catalyzed oxidation in their hemiacetal forms to give the (3S)-lactones directly. The hemiacetal oxidation is also stereoselective, preferring the (4S)-enantiomer. Substituent size at C-3 in the diols (C-4 in the hemiacetals) affects both the enantiotropic and enantiomeric specificity of the enzyme. Both types of stereospecificity diminish progressively for diol or hemiacetal substrates bearing large aliphatic (larger than Et) or aromatic substituents.
IT **71280-32-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 71280-32-5 CAPLUS
CN Pentanedioic acid, 3-(2-phenylethyl)- (9CI) (CA INDEX NAME)



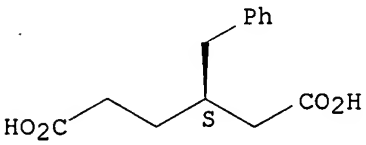
L19 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1979:167668 CAPLUS
DN 90:167668
TI Enzymes in organic synthesis. Influence of substrate structure on rates of horse liver alcohol dehydrogenase-catalyzed oxidoreductions
AU Irwin, Anthony J.; Lok, Kar P.; Huang, Ketz W. C.; Jones, J. Bryan
CS Dep. Chem., Univ. Toronto, Toronto, ON, Can.
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1978), (12), 1636-42
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal

LA English
OS CASREACT 90:167668
AB A kinetic study showed that horse-liver alc. dehydrogenase (HLADH)-catalyzed oxidoredns. of aliphatic alcs. and carbonyl substrates occur via an ordered Theorell-Chance mechanism. Coenzyme dissociation is largely rate determining for primary alc. and aldehyde oxidoredns., but not for secondary alcs. or ketones. The hydrophobic binding of a substrate at the active site is related to its relative reactivity. The degree of enantioselectivity achievable during HLADH-mediated transformations of racemates can be manipulated in some cases by varying the substrate concentration
IT **32386-49-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in pentanediol preparation)
RN 32386-49-5 CAPLUS
CN Pentanedioic acid, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



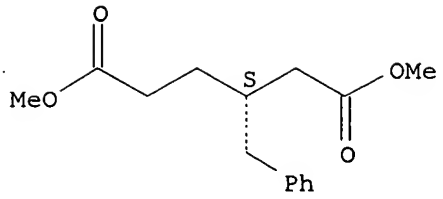
L19 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1976:542762 CAPLUS
DN 85:142762
TI A synthesis of optically active 3-benzyladipic acid and assignment of its absolute configuration
AU Ceder, Olof; Nilsson, Hans G.
CS Dep. Org. Chem., Univ. Goteborg, Goteborg, Swed.
SO Synthetic Communications (1976), 6(5), 381-6
CODEN: SYNCAV; ISSN: 0039-7911
DT Journal
LA English
AB (S)-(-)-3-benzyladipic acid was prepared via ozonolysis of (R)-(+)-3-cyclohexen-1-ylphenylmethane, which was obtained by subjecting (R)-(+)-3-cyclohexene-1-methanol to Fetizon oxidation and arylating the resultant (R)-(+)-3-cyclohexene-1-carboxaldehyde with PhLi.
IT **60631-78-9P 60631-79-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 60631-78-9 CAPLUS
CN Hexanedioic acid, 3-(phenylmethyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

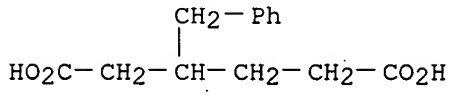


RN 60631-79-0 CAPLUS
CN Hexanedioic acid, 3-(phenylmethyl)-, dimethyl ester, (S)- (9CI) (CA INDEX NAME)

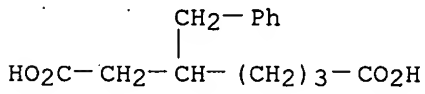
Absolute stereochemistry.



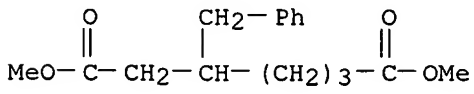
L19 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1975:592492 CAPLUS
DN 83:192492
TI β-Alkylalkanedioic acids from cycloalkenones via Michael alkylation-methoxycarbonylation
AU Salomon, Robert G.; Salomon, Mary F.
CS Dep. Chem., Case West. Reserve Univ., Cleveland, OH, USA
SO Journal of Organic Chemistry (1975), 40(10), 1488-92
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 83:192492
GI For diagram(s), see printed CA Issue.
AB Michael alkylation of 2-cycloalkenones with R2CuLi (R = Me, Bu, PhCH2, CH2:CH) and treatment with ClCO2Me gave the enol carbonates of cyclic β-keto esters (and in some cases the O-acylation products) which, with NaOH or NaOMe, underwent retro-Dieckmann cleavage to β-alkylalkanedioic acids or di-Me esters. The reactions were highly stereoselective, e.g., 5-methyl-2-cyclohexenone with Me2CuLi gave I which, with NaOMe-NaOH and then saponification, gave d,l-HO2CCH2CHMeCH2CHMeCH2CO2H. 2-Cyclopentenone, 2-cyclohexenone and several Me-substituted derivs., and 2-cycloheptenone were similarly treated.
IT **54576-12-4P 54576-17-9P 54576-18-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54576-12-4 CAPLUS
CN Hexanedioic acid, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 54576-17-9 CAPLUS
CN Heptanedioic acid, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 54576-18-0 CAPLUS
CN Heptanedioic acid, 3-(phenylmethyl)-, dimethyl ester (9CI) (CA INDEX NAME)



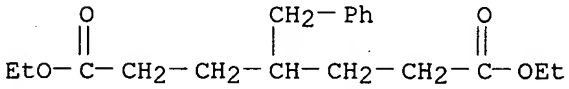
L19 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1967:453894 CAPLUS
DN 67:53894
TI Diethyl 4-benzylpimelate and the reduction of oxo esters
IN Chibnik, Sheldon
PA Mobil Oil Corp.
SO U.S., 2 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3317587		19670502	US	19631015

AB Saturated esters were prepared from the corresponding oxo esters RCOCH2-n-R1[CHR2(CHR3)mCO2R4]n (I), in which R is aryl or aromatic heterocyclic; R1 = H, Me, or Et; R2 = H or alkyl; R3 = H, Me, or Et; R4 = any alc. group normally forming an ester; m = 1 or 2; and n = 1 or 2. E.g., a stirred autoclave was charged with 320 parts di-Et 4-benzoylpimelate, 6 parts 5% Pd on alumina, 6 parts concentrated HCl, and 1500 parts EtOH. H was introduced into the autoclave at 60.5 psi. while the temperature was kept at 46° and, after 1.75 hrs., 2 moles H had been absorbed. The reaction mixture was filtered and then distilled at 155-8°/0.35 mm. to yield di-Et 4-benzylpimelate, n20D 1.4913. The products of this process are useful as plasticizers, solvents, and as monomers in the production of polymeric resins.

IT **16359-78-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16359-78-7 CAPLUS
CN Heptanedioic acid, 4-benzyl-, diethyl ester (8CI) (CA INDEX NAME)



L19 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1963:415380 CAPLUS
DN 59:15380
OREF 59:2724c-h
TI 2-(Substituted-benzyl)-1,3-propanedicarboxylic acids
IN Wilkinson, Raymond G.; Fields, Thomas L.
PA American Cyanamid Co.
SO 3 pp.
DT Patent
LA Unavailable

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3013069		19611212	US	19580715

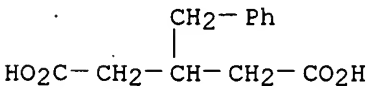
AB The title compds. (I) are useful for the preparation of 2-carboxymethyl- and 2-formylmethyl-4-oxotetrahydronaphthalenes and of poly-oxygenated cyclic compds. In an example, 94.0 g. 2-chloro-5-methoxy toluene is added to a mixture of 600 ml. CCl4, 117.4 g. N-bromosuccinimide, and 0.1 g. Bz2O2. The mixture is stirred and refluxed and addnl. 0.1-g. quantities of Bz2O2 are added after 1.5 and 18 hrs. After 21 hrs., the volume of solvent is reduced to about 250 ml. and the succinimide filtered off. The filtrate is washed thrice with 200 ml. H2O, dried, and filtered. The solvent is removed (vacuum) to yield 131.0 g. 2-chloro-5-methoxybenzyl bromide (II), m. 55.5-7.5° (20-40° petr. ether). II (131.0 g.) in 300 ml.

absolute EtOH is added over 1 hr. to a refluxing solution of 145 g. diethyl malonate (III) and 32.4 g. NaOMe in absolute EtOH. Refluxing is continued for an addnl. 2.5 hrs. and the mixture concentrated to approx. 1/2 volume NaBr is filtered off and the filtrate acidified slowly (HOAc). The solvent is removed (vacuum) and the residual oil dissolved in Et2O. The Et2O solution is washed with 200 ml. H2O, dried, and the Et2O and excess II distilled (vacuum). Diethyl 2-chloro-5-methoxybenzylmalonate (IV) (90 g.), b0.4 155-68°, n25D 1.5030, is collected. A solution of 105 g. IV in 360 ml. dry Et2O is added slowly with stirring to 19.5 g. LiAlH4 in 700 ml. dry Et2O. The mixture is stirred at reflux 4.5 hrs., then excess LiAlH4 is decomposed with EtOAc. The mixture is acidified with 6N HCl, washed, and kept over 70 ml. 5N NaOH. The Et2O layer is washed, dried, and concentrated Distillation at 0.1 mm. gives 64 g. 2-(2-chloro-5-methoxybenzyl)-1,3-propanediol (V), m. 41-6°. A solution of 100 g. V in 500 ml. C6H6 and 95 g. pyridine is cooled to 5°. MeSO2Cl (114 g.) is added over 0.5 hr. at 5-15°. The mixture is stirred at 5° for 16 hrs. The precipitated crystals are filtered off and washed with C6H6. The washings and filtrate are washed with 250 ml. N NaHCO3 then with 200 ml. H2O. The C6H6 layer is treated with active C, dried, and the solvent removed in vacuo to yield 135 g. 2-(2-chloro-5-methoxybenzyl)-1,3-propanediol bis(methanesulfonate) (VI), m. 75-7° (BuOH). A solution of 47.7 g. KCN in 230 ml. H2O is added to a solution of 135 g. VI in 690 ml. EtOH. The mixture is refluxed 4.5 hrs., 230 ml. 10N NaOH is added, and refluxing continued for an addnl. 16 hrs. The solution is concentrated to approx. 600 ml. by distillation at atmospheric pressure and then extracted with Et2O. The aqueous layer is treated with active C, filtered, and the filtrate cooled to 10° then acidified slowly with 200 ml. concentrated HCl. The precipitated solid is collected and dissolved in 350 ml. N NaHCO3. The solution is poured slowly into 200 ml. of 6N HCl to give 69 g. β-(2-chloro-5-methoxybenzyl)glutaric acid (VII), m. 117-18° (H2O-Me2CO). Also, V with p-MeC6H4SO2Cl gave 2-(2-chloro-5-methoxybenzyl)-1,3-propanediol bis(p-toluenesulfonate) which with NaCN gave VII. V with SOCl2 gave 2-(2-chloro-5-methoxybenzyl)-1,3-dichloropropane, which with NaI gave 2-(2-chloro-5-methoxybenzyl)-1,3-diiodopropane (VIII). VIII with NaCN gave β-(2-chloro-5-methoxybenzyl)glutaronitrile (IX), which, with alc. NaOH gave VII. Also, V with PBr3 gave 2-(2-chloro-5-methoxybenzyl)-1,3-dibromopropane (X). X with alc. NaCN gave IX, which with alc. NaOH gave VII.

IT **32386-49-5**, Glutaric acid, 3-benzyl- (derivs.)

RN 32386-49-5 CAPLUS

CN Pentanedioic acid, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



L19 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1956:27676 CAPLUS

DN 50:27676

OREF 50:5530f-h

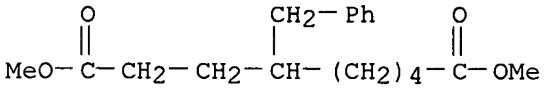
TI A new method for the preparation of long chain carboxylic acids. XI. Further examples of the course of Michael addition with 1,3-cyclohexanedione

AU Stetter, Hermann; Buntgen, Christa; Coenen, Marianne

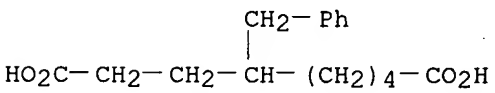
CS Univ. Bonn, Germany

SO Chemische Berichte (1955), 88, 77-81
CODEN: CHBEAM; ISSN: 0009-2940

DT Journal
LA Unavailable
OS CASREACT 50:27676
AB cf. C.A. 49, 14681i. $CH_2:CHCO_2Et$ (20 g.) and 14 g. 1-ethyl-2,6-cyclohexanedione, refluxed 20 hrs. with 0.5 g. Na and 30 cc. absolute EtOH gives 62% di-Et 4-oxo-3-ethylazelate (I), b3 170°. Similarly, 1-benzyl-2,6-cyclohexanedione gives 61% 3-benzyl analog (II), b5 214°. 1-Methyl-2,6-cyclohexanedione and Et maleate gives 62% tri-Et 4-oxo-3-methyl-1,2,7-heptanetricarboxylic acid (III), b5 214°. Dihydroresorcinol (11 g.) with 30 g. $CH_2:CHCO_2Et$ gives 64% di-Et 3-(2-carbethoxyethyl)-4-oxoazelate (IV), b2 187-9°. Reduction of I, II, III, and IV by heating with $N_2H_4.H_2O$, NaOH, and diethylene glycol yields 88% γ-ethylazelaic acid (di-Me ester, b2 125°), 86% γ-benzylazelaic acid (di-Me ester, b2 192°), 52% 3-methyl-1,2,7-heptanetricarboxylic acid (tri-Me ester, b2 176°), and 75% 3-(2-carboxyethyl)azelaic acid (tri-Me ester, b2 159°), resp.
IT **859987-61-4**, Nonanedioic acid, 4-benzyl-, dimethyl ester
859987-62-5, Nonanedioic acid, 4-benzyl-
(preparation of)
RN 859987-61-4 CAPLUS
CN Nonanedioic acid, 4-benzyl-, dimethyl ester (5CI) (CA INDEX NAME)



RN 859987-62-5 CAPLUS
CN Nonanedioic acid, 4-benzyl- (5CI) (CA INDEX NAME)



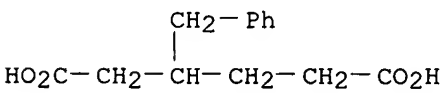
L19 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1928:9614 CAPLUS
DN 22:9614
OREF 22:1153d-i,1154a
TI The relative ease of formation of rings. I
AU v. Braun, Julius; Bayer, Otto; Cassel, Leberecht
SO Ber. (1927), 60B, 2602-9
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB In a compound in which the formation of 2 rings is possible, a determination of which ring is formed exclusively or predominantly should afford a suitable basis for comparing the relative ease of formation of the 2 cyclic structures. The only necessary condition is that the atomic groups concerned in the ring formation must be of absolutely the same character. A study of this problem on a broad exptl. basis has been undertaken; in the present paper are given 2 examples of the method of attack: determination of the relative ease of formation of 4- and 5-membered rings on a C_6H_6 nucleus and of tetrahydro- and homotetrahydroisoquinoline rings. $PhCH_2CH(CH_2COCl)CH_2CH_2COCl$ (I), which might form either II or III by ring closure, tends to form the ring exclusively in the first direction, for when the C:O group in the resulting acid is replaced by CH_2 there is formed an acid (IV) of the hydronaphthalene series, as shown by its

thermal decomposition to C10H8. Ph(PhCH2)CHCH2N(SO2C6H4Me)-CH2CO2H (V) with P2O5 yields a perfectly homogeneous compound (VI) giving on saponification and dehydrogenation an entirely homogeneous 4-benzylisoquinoline, showing that the tendency to ring formation is beyond doubt greater with tetrahydroisoquinoline than with the asym. ring homolog. p-Benzylcyclohexanol (VII), from p-PhCH2C6H4OH with H and Ni somewhat above 200°, b14 171°, consists of a mixture of 2 stereoisomers (on long standing at 0°, about 50% solidifies and, after carefully pressing, m. 35-40°); phenylurethan, m. 154-7°. p-Benzylcyclohexanone, from VII with CrO3-AcOH, b14 165-6°, m. 46-7°; semicarbazone, m. 145-7°. p-Hexahydrobenzylcyclohexanol, obtained by further reduction of VII, b14 158°; phenylurethan, m. 153-5°. Hexahydrobenzylcyclohexanone, b14 155°. β-Benzyladipic acid, from VII in 1.6 mols. KOH with the calculated amount of very dilute (0.03%) KMnO4 at 0° (yield, 35% starting with 5 g. VII, only 20% starting with 15 g. VII), m. 110-1°, cannot be distilled without decomposition, losing H2O and forming the anhydride, b16 245-50°, m. 90°; Et ester, b14 220°. The chloride (I), which cannot be distilled without decomposition, gives with 2 mols. AlCl3 on the H2O bath 55% of ac-α-tetralone-γ-propionic acid (II), m. 136-7°; semicarbazone, m. 260°; oxime, m. 148°; phenylhydrazone, m. 152°, faintly reddish. II by the Clemmensen method gives almost 70% ac-β-tetralylpropionic acid (IV), m. 73°; Et ester, b14 188-90°, d422 1.040, nD22 1.5153; amide, m. 130°. Ph(PhCH2)CHCH2NH2, b12 182°, is obtained in 80% yield from PhCH:CPhCN with Ni and H2 (best without a solvent) at 210°; its Bz derivative, b11 280°, yields with 1 mol. PCl5 25% of β,γ-diphenylpropyl chloride, b11 150°, faintly yellow. N-p-Toluenesulfonyl-N-[β-benzyl-β-phenylethyl]glycine (V), from the above amine treated in C6H6 with 0.5 mol. BrCH2CO2Et, shaken out with very dilute HCl, evaporated twice with concentrated HCl to saponification the ester Ph(PhCH2)CHCH2NHCH2CO2Et, made alkaline, extracted with Et2O and treated with MeC6H4SO2Cl, m. 135°, gives in boiling xylene with 2.5 parts P2O5 almost 100% of the p-toluenesulfonyl derivative (VI), m. 158-60°, of 4-benzyl-1,2,3,4-tetrahydroisoquinoline, b15 204-5°, m. 49-50° (HCl salt, m. 155°; picrate, m. 150°; Ac derivative, oily; NO derivative, m. 100°; phenylthiourea, m. 166°; quaternary methiodide, m. 186°).

IT **54576-12-4**, Adipic acid, β-benzyl- **860738-55-2**, Adipic acid, β-benzyl-, diethyl ester
(preparation of)

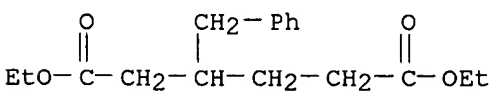
RN 54576-12-4 CAPLUS

CN Hexanedioic acid, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 860738-55-2 CAPLUS

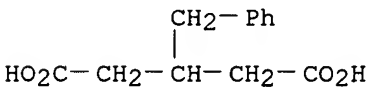
CN Adipic acid, β-benzyl-, diethyl ester (3CI) (CA INDEX NAME)



L19 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1922:24685 CAPLUS
DN 16:24685
OREF 16:4203h-i,4204a
TI Formation of derivatives of tetrahydronaphthalene from γ-phenyl fatty acids. II
AU Stevenson, Arnold; Thorpe, Jocelyn Field
SO Journal of the Chemical Society, Transactions (1922), 121, 1717-22
CODEN: JCHTA3; ISSN: 0368-1645
DT Journal
LA Unavailable
AB cf. C. A. 15, 1279. The earlier work has been continued for the purpose of investigating the effect of substitution at different positions on the side chain, as a part of the general problem of the stereochem, configuration of the C6H6 nucleus. PhCH2CHO may be stabilized (prevented from polymerizing) by the addition of about 2 times its weight of absolute EtOH.

Condensation with CNCH2CONH2 gave a 10% yield of PhCH2CH[CH(CN)CONH2]2 (A), m. 249° (decomposition), though the major portion of the product is the α-cyano-γ-phenylcrotonic amide, CH2PhCH:C(CN)CONH2, needles, m. 207°. β-Benzylglutaric acid (B), PhCH2CH(CH2CO2H)2, results by the hydrolysis of A with concentrated HCl or dilute H2SO4, stout prisms, m. 99-101°. Concentrated H2SO4 at room temperature transforms B into ac-1-ketotetrahydronaphthalene-3-acetic acid, prisms from C6H6, m. 110-1°. Semicarbazone, m. 238°. Oxidation with alkaline KMnO4, gave C6H4(CO2H)2. Attempts to carry out a regulated oxidation, using 1% KMnO4 at 10°, gave only a tar and unchanged acid.

IT **32386-49-5**, Glutaric acid, β-benzyl-
(preparation of)
RN 32386-49-5 CAPLUS
CN Pentanedioic acid, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



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